

9th December, 2019

09:00 Registration
09:30 Introduction to Training Programme – B Singh
09:35 Welcome –Director, CSIR-IMTECH
09:40 Bioinformatics Centre at IMTECH: Highlights and Introduction of Speaker – S Srikrishna
09:45 Protein structure to Bioinformatics to Drug Discovery– TP Singh
10:30 High Tea
11:00 Computational analysis of protein-protein interactions – R Sowdhamini
12:00 Revisiting India's pride: The Ramachandran map - all over again – N Srinivasan
13:00 Lunch
14:00 Bridging the islands of protein families in sequence space using artificial sequences – N Srinivasan
14:45 Introduction to Linux/UNIX – C Sharma/A Yadav
15:30 Tea
16:00 Installation of Linux – Demo -Hands on Session – C Sharma/A Yadav
20:00 Dinner

10th December, 2019

09:30 A Talk by K Gopal
10:15 Demo and Hands on session – K Gopal
11:00 Tea
11:30 Merging low resolution (SAXS) information with low confidence (MD or modeling) data to understand proteins - Ashish
12:15 Landscape of intra-chain domain-domain Interfaces – SB Pandit
13:00 Lunch
14:00 Demo and Hands on session – SB Pandit
16:00 Tea
16:30 Demo and Hands on Session – Ashish
20:00 Dinner

11th December, 2019

09:30 Computational mutagenesis reveals amino acids that play a role in the entry of ion in active site of DHBPS: Mechanistic insights from MD Simulations – B Singh
10:15 Modeling Protein Structures – Demo cum-Lecture– S Beriwal
11:00 Tea
11:30 Demo and Hands on Session – B Singh
12:15 *In Silico* Investigations of Antimalarial Activities of Artemisinin: A *Bi-radical* Perspective – Ehesan Ali
13:00 Lunch

14:00 Demo and Hands on Session – Ehesan Ali
15:30 Tea
16:00 Demo and Hands on Session – Ehesan Ali
20:00 Dinner

12th December, 2019

09:30 Quantitative structure–activity relationship (QSAR) models development using machine learning for antiviral drug discover Talk - M Kumar
10:15 Application of cheminformatics in drug discovery– A Nargotra
11:00 Tea
11:30 Protein Sequence Structure function Analysis: Noteworthy examples of Zn finger proteins by S Srikrishna
12:15 Demo and Hands on session – A Nargotra
13:00 Lunch
14:00 Tour to IMTECH facilities- Virtual Reality and 3D Printing – Demo- S Srikrishna
15:30 Tea
16:00 Demo and Hands on Session – A Nargotra
20:00 Dinner

13th December, 2019

09:30 Dynamic Hybrid Pharmacophore Approach for Discovery of New Drugs - A Bhardwaj
10:30 Combining bioinformatics and experimental approaches to understand "protein sequence to function and disease" relationships - Beena Krishnan
11:15 Tea
11:45 Structure-Toxicity link of protein aggregates in human diseases - A Kumar
13:00 Lunch
14:30 Interactive Session
15:00 Valedictory Function
15:30 Tea

Note:

- Registration of training program will take place at reception area of IMTECH-Main building.
- Talks will be held in Crystal Room, GNR Protein Centre except the inaugural function. Demo-Hands-on Session will be in user lab, first floor, GNR protein Centre.
- Breakfast and dinner will be served in the Guest House for participants.
- Lunch will be served all days in the cafeteria, unless otherwise notified.